CellML Specification 1.1 Draft — 6 November 2002

A Using The CellML 1.0 DTD

A.1 Introduction

This section contains some recommendations on the use and referencing of the CellML 1.1 DTD, the full text of which is given in Appendix A.6. The document rules and processor behaviour described in this section are not required in valid CellML documents and from CellML conformant processing software, respectively.

A.2 The CellML DOCTYPE declaration

CellML documents may reference the version of the CellML 1.1 DTD maintained on the CellML website with a DOCTYPE declarations of the following form:

```
<!DOCTYPE model SYSTEM "http://www.cellml.org/cellml/cellml_1_1.dtd">
```

"model" may be changed to match the root element of the CellML document.

CellML document authors may change the value of the system identifier to point to a copy of the DTD cached on a local filesystem if this is available. This specification does not define a public identifier for CellML 1.0. For interoperability, CellML document authors should not define one unless specifically needed for a parser that makes use of SGML catalog files.

A.3 CellML without a DTD

CellML documents are not required to contain a DOCTYPE declaration. In the absence of a DTD, CellML processing software needs to take into account the following important points:

- All **cmeta**: id attributes are of type ID.
- All id attributes on MathML elements are of type ID.

The CellML DTD does not define the default values for CellML attributes that are defined in the specification. With or without a DTD, CellML processing software is responsible for setting these values, if not specified.

A.4 Use of MathML within CellML

The CellML 1.1 DTD can be used in conjunction with the <u>MathML 2.0 DTD¹</u> to validate any MathML content within a CellML document. The CellML DTD contains a reference to the MathML 2.0 DTD, which is maintained at the <u>World Wide Web Consortium's website²</u>, inside a conditional section, which by default is not included in the CellML DTD. CellML document authors may cause the conditional section to be included by setting the value of the "use_mathml_dtd" entity to "INCLUDE" inside the internal subset of their CellML document, as shown below:

¹http://www.w3.org/TR/MathML2/dtd/mathml2.dtd

²http://www.w3.org/

```
<!DOCTYPE model SYSTEM "http://www.cellml.org/cellml/cellml_1_1.dtd" [
    <!ENTITY % use_mathml_dtd "INCLUDE">
]>
```

If copies of both the CellML 1.1 DTD and the MathML 2.0 DTD are available on the local filesystem, it is possible to conveniently override the reference to the MathML 2.0 DTD by setting the value of the "mathml_dtd_path" entity to the appropriate relative path from the CellML DTD to the MathML DTD, as shown below:

```
<!DOCTYPE model SYSTEM "/my/local/copy/of/the/cellml_1_1.dtd" [
    <!ENTITY % mathml_dtd_path "'relative/path/to/mathml2.dtd'">
    <!ENTITY % use_mathml_dtd "INCLUDE">
]>
```

The MathML 2.0 DTD is not on the CellML website, so DOCTYPE declarations of this form will fail when referencing the DTD on the CellML website. The MathML 2.0 DTDs are available as a ZIP archive, a link to which is given in <u>Appendix A.6 of the MathML 2.0 Recommendation</u>³.

The CellML specification requires a **cellml:units** attribute to be defined on all **<mathml:cn>** elements (where the **cellml** and **mathml** prefixes are mapped to the URIs for the CellML and MathML namespaces, respectively). For this reason, the conditional section of the CellML DTD in which the MathML DTD is referenced also redeclares the list of attributes on the **<mathml:cn>** element to include the **cellml:units** attribute. This will prevent XML parsers from finding errors when validating valid CellML documents against the MathML DTD.

A.5 Treatment of namespaces

In Section 2.2.2⁴, it was suggested that the root element of a CellML document set the default namespace and map the cellml prefix to the CellML namespace URI. Use of unprefixed element names (i.e., default namespaces) is encouraged to ensure DTD-based validation will work correctly. The CellML 1.1 DTD defines three optional attributes on every CellML element that can be used to set namespaces where necessary. These are xmlns, xmlns:cellml and xmlns:cmeta.

A.6 The CellML 1.1 DTD

The CellML 1.1 DTD is available at the following URI:

http://www.cellml.org/cellml/cellml_1_1.dtd

The CellML 1.1 DTD does not attempt to declare or reference declarations for the metadata framework elements in the RDF namespace. It also doesn't declare the default values of any of the attributes on the CellML elements.

For convenient reference, the text of the DTD is given below.

```
<!--
FILE : cellml_1_1.dtd
CREATED : 26 August 2002
```

³http://www.w3.org/TR/2001/REC-MathML2-20010221/appendixa.html#parsing_dtd

⁴http://www.cellml.org/public/specification/cellml_specification.html#sec_fundamentals_namespaces

```
LAST MODIFIED : 29 September 2003
AUTHOR : Autumn A. Cuellar (a.cuellar@auckland.ac.nz)
         Warren Hedley
         The Bioengineering Institute
         The University of Auckland
DESCRIPTION : This document contains a DTD corresponding to the syntax rules
  defined in the Developer's Specification for CellML 1.1. This
  specification is available at
    http://www.cellml.org/private/specification/unstable/index.html
SYSTEM IDENTIFIER : http://www.cellml.org/cellml/cellml_1_1.dtd
COPYRIGHT : (2002) Bioengineering Institute, The University of Auckland.
-->
<!ENTITY % use_mathml_dtd "IGNORE">
<![%use_mathml_dtd;[
  <!ENTITY % mathml-charent.module "IGNORE">
  <!ENTITY % mathml_dtd_path
    "'http://www.w3.org/TR/MathML2/dtd/mathml2.dtd'">
  <!ENTITY % mathml_dtd PUBLIC "-//W3C//DTD MathML 2.0//EN"</pre>
    %mathml_dtd_path;>
  %mathml dtd;
  <!ATTLIST %cn.qname;
    %MATHML.Common.attrib;
    %att-type;
    %att-base;
    %att-definition;
    %att-encoding;
    cellml:units
                      CDATA
                                      #REQUIRED
  >
]]>
<!ENTITY % cellml_common_attributes "
                                      #IMPLIED
  xmlns
                      CDATA
  xmlns:cellml
                      CDATA
                                      #IMPLIED
  xmlns:cmeta
                      CDATA
                                      #IMPLIED
                      TD
                                      #IMPLIED
  cmeta:id
115
<!ELEMENT model (import | units | component | group | connection)*>
<!ATTLIST model
  %cellml_common_attributes;
                                      #REQUIRED
  name
                      CDATA
>
<!ELEMENT import (units | component)*>
<!ATTLIST import
  %cellml_common_attributes;
  xlink:type
                                      #FIXED "simple"
                      (simple)
                                      #REQUIRED
  xlink:href
                      CDATA
>
<!ELEMENT component (units | variable | reaction | math)*>
<!ATTLIST component
```

```
%cellml_common_attributes;
                                     #REQUIRED
 name
                    CDATA
 component_ref
                     CDATA
                                     #IMPLIED
>
<!ELEMENT variable EMPTY>
<!ATTLIST variable
 %cellml_common_attributes;
                                     #REQUIRED
 name
                     CDATA
                     (in|out|none) #IMPLIED
 public interface
 private_interface (in out none) #IMPLIED
 units
                     CDATA
                                     #REQUIRED
 initial_value
                     CDATA
                                    #IMPLIED
>
<!ELEMENT connection (map_components | map_variables+)>
<!ATTLIST connection
  %cellml common attributes;
>
<!ELEMENT map_components EMPTY>
<!ATTLIST map_components
 %cellml_common_attributes;
                                     #REQUIRED
 component_1
                   CDATA
 component_2
                     CDATA
                                     #REQUIRED
>
<!ELEMENT map_variables EMPTY>
<!ATTLIST map variables
 %cellml_common_attributes;
                                     #REQUIRED
 variable 1
                     CDATA
                                     #REQUIRED
 variable_2
                     CDATA
>
<!ELEMENT units (unit*)>
<!ATTLIST units
 %cellml_common_attributes;
                                     #REQUIRED
 name
                     CDATA
 units_ref
                     CDATA
                                     #IMPLIED
 base_units
                    (yes|no)
                                     #IMPLIED
>
<!ELEMENT unit EMPTY>
<!ATTLIST unit
 %cellml_common_attributes;
                                     #IMPLIED
 multiplier
                    CDATA
 prefix
                     CDATA
                                     #IMPLIED
 units
                     CDATA
                                     #REQUIRED
 exponent
                     CDATA
                                     #IMPLIED
 offset
                     CDATA
                                     #IMPLIED
>
<!ELEMENT group (relationship_ref | component_ref)+>
<!ATTLIST group
  %cellml_common_attributes;
>
<!ELEMENT relationship_ref EMPTY>
<!ATTLIST relationship_ref
```

```
%cellml_common_attributes;
  relationship (encapsulation containment) #IMPLIED
>
<!ELEMENT component_ref (component_ref*)>
<!ATTLIST component_ref
  %cellml_common_attributes;
  component
                     CDATA
                                     #REQUIRED
>
<!ELEMENT reaction (variable_ref+)>
<!ATTLIST reaction
 %cellml_common_attributes;
  reversible
                     (yes no)
                                     #IMPLIED
>
<!ELEMENT variable_ref (role+)>
<!ATTLIST variable_ref
  %cellml_common_attributes;
                                     #REQUIRED
  variable
                    CDATA
>
<!ELEMENT role (math?)>
<!ATTLIST role
  %cellml_common_attributes;
  role (reactant|product|activator|catalyst|inhibitor|modifier|rate) #REQUIRED
  direction (forward|backward|both) #IMPLIED
  delta_variable
                   CDATA
                                     #IMPLIED
  stoichiometry
                    CDATA
                                     #IMPLIED
>
```

B Scripting functionality in CellML

B.1 Introduction

MathML can be extended by defining new operators, the behaviour of which is not defined in MathML. These operators could be used to call functions implemented in software (i.e., implicitly) or defined using a scripting language (i.e., explicitly). CellML 1.1 does not require processing software to implement support for scripting functionality. This section contains some recommendations on best practices for adding scripting functionality to CellML.

For the purposes of this discussion, it is assumed that scripting functionality will be implemented via function calls. Software that extends the functionality of MathML in other ways should extrapolate these recommendations as appropriate.

B.2 Availability of scripts

Functions referenced in a CellML document that are defined using non-MathML syntax should be identified by, and accessible via, a URI. A function could, for instance, be accessible via HTTP from a database using a CGI script that takes an SQL expression as an argument.

B.3 Embedding scripts in CellML

Functions should be defined within elements in an application-specific extension namespace, if the functions are embedded within CellML documents. If the embedded script is only referenced by a single component, the script should be defined within the corresponding **<cellml:component>** element. If the embedded script is referenced by more than one component, the script should be defined within the **<cellml:model>** element.

B.4 Preferred scripting language

Implementors considering adding scripting functionality to CellML processing software are encouraged to use ECMAScript. It is anticipated that, if scripting functionality is officially endorsed by a future version of CellML, ECMAScript will be the scripting language that processing software is required to implement. ECMAScript is the recommended language because it is simple, standardised, and open source interpreting libraries are freely available.

<u>ECMA⁵</u> is an international industry association that develops standards in information and communication for the European union. ECMA took the scripting language that <u>Netscape⁶</u> developed for adding interactive content to its web browser and developed the formal language specification <u>ECMA-262 (ECMAScript</u> Language Specification)⁷.

B.5 Referencing scripts from MathML

The <u>MathML 2.0 Recommendation</u>⁸ defines a **<mathml:csymbol>** element for referencing mathematical symbols and constructs that are not defined by MathML. This element should be used for referencing functions defined using non-MathML syntax from within blocks of MathML. Processing software should take into account the following recommendations regarding the use of the **<mathml:csymbol>** element for this purpose.

⁵http://www.ecma.ch/

⁶http://www.netscape.com/

⁷http://www.ecma.ch/ecma1/STAND/ECMA-262.HTM

⁸http://www.w3.org/TR/2001/REC-MathML2-20010221

B.5.1 The <mathml:csymbol>element

1. Recommended use of the <mathml:csymbol> element

• The <mathml:csymbol> element should only appear as the first child element within a <mathml:apply> element.

[A **<mathml:csymbol>** element should only be used as an operator, which is "applied" to some arguments.]

• After leading and trailing whitespace is removed, the content of a <mathml:csymbol> element must be a valid CellML identifier as discussed in <u>Section 2.2.1</u>⁹. This identifier must accurately represent the external function referenced.

[The content of a **<mathml:csymbol>** element should preferably be a human-readable identifier for the external function. If the function is defined using a common scripting or programming language, then this identifier should be the name of the function.]

• Each <mathml:csymbol> element should define a definitionURL and an encoding attribute.

2. Recommended use of the mathml:definitionURL attribute

• The value of the **definitionURL** attribute should be a valid URI that identifies a single resource containing the definition of the external function.

3. Recommended use of the mathml:encoding attribute

• The value of the **encoding** attribute should indicate to processing software the format of the externally defined function.

[In the version of CellML that describes how external functions are to be defined within the CellML framework, the **encoding** attribute will be moved into the CellML namespace and will be required to take a value from a controlled vocabulary.]

B.6 Effects of scripts

Functions must be side-effect free. That is, a function must not assign values to variables that are not local to that function. In particular, functions must not alter the values of their arguments or global variables.

⁹http://www.cellml.org/public/specification/cellml_specification.html#sec_fundamentals_identifiers

C Advanced Units Functionality

C.1 Introduction

CellML 1.1 lays the foundations of a flexible and robust system for the association of units with variables and constants in cellular models. However, it does not require software to make use of the units information contained in CellML documents. This section presents algorithms and examples demonstrating some of the advanced features related to units that CellML processing software might choose to offer modellers. For interoperability, CellML processing software that includes these features should achieve the same results as the algorithms described here, although the exact implementation may differ.

C.2 Terminology

C.2.1 Equivalence of units references

Two units references are considered equivalent if they satisfy one of the following criteria:

- They reference the same units definition from the standard dictionary.
- They reference the same units definition in the current **<component>** element.
- They reference the same units definition in the current <model> element, where that units definition is not superseded by a units definition with the same name in the current <component> element.

C.2.2 Dimensional equivalence of units definitions

Two units definitions have dimensional equivalence if, when each is recursively expanded and simplified until left with nothing but products of SI and user-defined base units:

- the expanded form of each units definition consists of the same set of base units, and
- the exponent on each base unit is identical in each expanded units definition.

Algorithms for the expansion and simplification of units definitions are given in Appendix C.3.4 and Appendix C.3.1, respectively.

C.3 Algorithms

C.3.1 Simplification of units definitions

It is frequently convenient to be able to simplify a units definition, where this units definition is the result of the application of some mathematical operator to terms which have units associated with them. These operators include the **<times>**, **<divide>** and **<diff>** operators.

The simplification of a units definition is an iterative process in which the number of other units definitions referenced is systematically reduced. References to units definitions may be removed in the following cases:

- If two units references are equivalent (as defined in Appendix C.2.1) and have exponents with equal and opposite value, then they may be replaced by a reference to **dimensionless**.
- If two units references are equivalent (as defined in Appendix C.2.1) then they may be replaced with a single units reference to the same units, where the exponent associated with that units reference is the sum of the exponents on the original two units references.

- If a units definition references **dimensionless** one or more times in addition to some other units, any references to **dimensionless** may be removed.
- If a units definition references **dimensionless** one or more times and references no other units, the definition may be replaced with **dimensionless**.

The above rules only allow the removal of units references that are equivalent as defined in Appendix C.2.1. This scheme would not allow references to identical units definitions in two different components to be cancelled and removed, because the references would not satisfy the equivalence criteria.

C.3.2 Units-based restrictions on the use of MathML operators

This section describes restrictions on the units associated with a collection of terms to which each MathML operator in the CellML set (defined in Section 4.2.3¹⁰) can be applied. For instance, the **<mathml:plus>** operator can only be applied to terms that have dimensionally equivalent units. The restrictions invalidate the application of certain MathML operators to certain collections of terms based on their units, and are used in equation dimension checking, as described in Appendix C.3.6.

The restrictions are given in Table 5. The <mathml:root>, <mathml:diff> and <mathml:log> elements all take qualifiers, in addition to operands.

C.3.3 Applying operators to units definitions

The section defines the units resulting from the application of MathML operators to a collection of terms, each with known units. This is needed for units definition conversion and equation dimension checking, as described in Appendix C.3.5 and Appendix C.3.6, respectively. The units on each of the terms in the collection must satisfy the restrictions defined in Appendix C.3.2 for the current operator.

The full set of units calculation rules are described in Table 6.

C.3.4 Expansion of units definitions

This section presents the recommended algorithm for expanding a given units definition into an expression that relates the defined units to only SI and user-defined base units. This algorithm may be used in the conversion of units definitions and equation dimension checking, algorithms for which are defined in Appendix C.3.5 and Appendix C.3.6, respectively. Examples of the expansion of units definitions are given in Appendix C.4.2.

The specific steps in the algorithm depend on whether the units definition to be expanded is simple or complex, as defined in Section $5.2.2^{12}$. Both derivations use recursive methods. At each step, any units that are not base units are replaced with expansions based on the appropriate definition.

Expansion of simple units definitions

The formula relating a variable x_U with units of **U** (where **U** are simple units), to a variable x_1 with units of **u**₁ (the subunits referenced by the **units** attribute on the **<unit>** element inside the units definition for **U**), is given in Equation (9). This is based on the simple units definition formula given in Equation (??).

$$x_U \begin{bmatrix} \mathbf{U} \end{bmatrix} = (m_1 p_1) \begin{bmatrix} \mathbf{U} \\ \mathbf{u}_1 \end{bmatrix} x_1 \begin{bmatrix} \mathbf{u}_1 \end{bmatrix} + o_1 \begin{bmatrix} \mathbf{U} \end{bmatrix}$$
(9)

 m_1 , p_1 and o_1 correspond to the **multiplier**, **prefix** and **offset** attributes on the **<unit>** element, respectively.

¹⁰http://www.cellml.org/public/specification/cellml_specification.html#sec_math_cellml_subset

¹²http://www.cellml.org/public/specification/cellml_specification.html#sec_units_user_defined_units

Restrictions
There are no restrictions on the units of
operands for these operators.
These operators, if applied to more than
one operand, require all of their operands
to have either equivalent units references,
as defined in Appendix C.2.1, or to refer-
ence units that have dimensional equiva-
lence, as defined in Appendix C.2.2.
These operators require their operands to
have units of cellml:boolean , as de-
fined in Section $5.5.2^{11}$.
These operators require their operands to
have units of dimensionless .
This is a binary arithmetic operator. Its
first operand may have any units, and
its second operand must have units of
dimensionless.
This is a qualified unary operator. Its
operand may have any units. The
value of the <degree> qualifier ele- ment, if present, must have units of</degree>
dimensionless.
This is a qualified unary opera-
tor. Its operand must have units of
dimensionless. The value of the
<pre><logbase> qualifier element, if present,</logbase></pre>
must have units of dimensionless .
The operand of this operator and the
value of the <bvar></bvar> qualifier element, if
present, may have any units. The value
of a <degree></degree> qualifier element within
the <bvar></bvar> qualifier element, if present,

 TABLE 5: The restrictions on the units associated with operands and qualifiers for each MathML operator.
 All elements in this table are in the MathML namespace.

Operator	Result Units
<pre><eq>, <neq>, <gt>, <lt>, <geq>,</geq></lt></gt></neq></eq></pre>	The result of these operators has units of
<leq>, <and>, <or>, <xor>, <not></not></xor></or></and></leq>	cellml:boolean.
<pre><exp>, <ln>, <log>, <factorial>,</factorial></log></ln></exp></pre>	The result of these operators has units of
<pre><sin>, <cos>, <tan>, <sec>,</sec></tan></cos></sin></pre>	dimensionless.
< csc >, $< cot >$, $< sinh >$, $< cosh >$,	
< tanh>, < sech>, < csch>,	
<coth>, <arcsin>, <arccos>,</arccos></arcsin></coth>	
<pre><arctan>, <arccosh>, <arccot>,</arccot></arccosh></arctan></pre>	
<pre><arccoth>, <arccsc>, <arccsch>,</arccsch></arccsc></arccoth></pre>	
<pre><arcsec>, <arcsech>, <arcsinh>,</arcsinh></arcsech></arcsec></pre>	
<arctanh></arctanh>	
<plus>, <minus>, <abs>, <floor>,</floor></abs></minus></plus>	The result of these operators has the same
<ceiling></ceiling>	units as the operands.
<times></times>	The result of this operator has units
	that are the product of the units on the
	operands. This product may be simpli-
	fied according to the rules outlined in Appendix C.3.1.
<divide></divide>	The result of this operator has units that
	are the quotient of the units on the first
	and second operands. This quotient may
	be simplified according to the rules out-
	lined in Appendix C.3.1.
<power></power>	The result of this operator has units
-	that are the units on the first operand
	raised to the power of the second
	operand. If the first operand has units
	of dimensionless, the result also has
	units of dimensionless .
<root></root>	The result of this operator has units that
	are the units on the first operand raised to
	one over the value of the <degree></degree> qual-
	ifier element (the default value of which
	is 2.0). If the first operand has units
	of dimensionless , the result also has
	units of dimensionless.
<diff></diff>	The result of this operator has units that
	are the quotient of the units of the operand
	over the units of the term in the <bvar></bvar>
	qualifier element raised to the value of
	the <degree></degree> qualifier element inside the <bvar></bvar> qualifier element (the default
	value of which is 1.0). This quotient may
	be simplified according to the rules out-
	lined in Appendix C.3.1.

TABLE 6: The units of the result after applying each MathML operator to a collection of terms, where the units on those terms satisfy the restrictions in Appendix C.3.2. All elements in this table are in the MathML namespace.

The formula relating a variable with units of u_1 to its subunits u_2 , as referenced in the units definition for u_1 , is given in Equation (10).

$$x_{1} [\mathbf{u}_{1}] = (m_{2} p_{2}) \left[\frac{\mathbf{u}_{1}}{\mathbf{u}_{2}} \right] x_{2} [\mathbf{u}_{2}] + o_{2} [\mathbf{u}_{1}]$$
(10)

Equation (10) can be substituted into Equation (9) to give Equation (11).

$$x_{U} [\mathbf{U}] = (m_{1} p_{1}) \left[\frac{\mathbf{U}}{\mathbf{u}_{1}}\right] \left((m_{2} p_{2}) \left[\frac{\mathbf{u}_{1}}{\mathbf{u}_{2}}\right] x_{2} [\mathbf{u}_{2}] + o_{2} [\mathbf{u}_{1}]\right) + o_{1} [\mathbf{U}]$$
(11)

The expression defining each new set of units in terms of its subunits can be substituted into the current expression recursively until an expression is reached that relates x_U to x_n with units u_n , which are SI or user-defined base units. At this point expansion stops, and the resulting expression can be simplified. This simplification combines multiplier, prefix and offset terms and combines their units based on the rules defined in Appendix C.3.3. The result is an expression of the form given in Equation (12).

$$x_{U} \begin{bmatrix} \mathbf{U} \end{bmatrix} = m_{t} \begin{bmatrix} \mathbf{U} \\ \mathbf{u}_{n} \end{bmatrix} x_{n} \begin{bmatrix} \mathbf{u}_{n} \end{bmatrix} + o_{t} \begin{bmatrix} \mathbf{U} \end{bmatrix}$$
(12)

The values of m_t and o_t are given by Equation (13) and Equation (14), respectively.

$$m_t = (m_1 p_1) \dots (m_n p_n)$$

$$(13)$$

$$o_t = m_1 p_1 \left(o_2 + m_2 p_2 \left(o_3 + \dots + m_{n-1} p_{n-1} o_n \right) \right)$$
(14)

Expansion of complex units definitions

The formula relating a variable x_U with complex units **u** to a variable x_A with units that are the product of the subunits referenced in the units definition for **u** is given in Equation (15). This is based on the complex units definition formula given in Equation (??).

$$x_{U} \begin{bmatrix} \mathbf{U} \end{bmatrix} = (m_{A1} \dots m_{An} p_{A1}^{e_{A1}} \dots p_{An}^{e_{An}}) \begin{bmatrix} \mathbf{U} \\ \mathbf{u}_{A1}^{e_{A1}} \dots \mathbf{u}_{An}^{e_{An}} \end{bmatrix} x_{A} \begin{bmatrix} \mathbf{u}_{A1}^{e_{A1}} \dots \mathbf{u}_{An}^{e_{An}} \end{bmatrix}$$
(15)

The m_{Ai} , p_{Ai} , \mathbf{u}_{Ai} and e_{Ai} refer to the values of the **multiplier**, **prefix**, **units** and **exponent** attributes on the *i*-th **<unit>** element inside the units definition for U, respectively. If, at the first step, the *c*-th set of units referenced is not SI or user-defined base units, the formula relating \mathbf{u}_{Ac} to the *c*-th set of units referenced to its subunits is given in Equation (16).

$$x_{C} [\mathbf{u}_{Ac}] = (m_{B1} \dots m_{Bn} p_{B1}^{e_{B1}} \dots p_{Bn}^{e_{Bn}}) \left[\frac{U}{\mathbf{u}_{B1}^{e_{B1}} \dots \mathbf{u}_{Bn}^{e_{Bn}}} \right] x_{B} [\mathbf{u}_{B1}^{e_{B1}} \dots \mathbf{u}_{Bn}^{e_{Bn}}]$$
(16)

Note that if u_{Ac} is a simple units definition, then the right hand side of Equation (16) will take the form of a simple units definition, but *without the constant offset term*.

An expansion for x_A that incorporates the expansion for \mathbf{u}_{Ac} is obtained by multiplying both sides of Equation (16) by unitary coefficients with units of the product of all of the units referenced on the right hand side of Equation (15) with the exception of \mathbf{u}_{Ac} . Expansion of units definitions involves constructing expansions for the variable on the right hand side. The expansion continues recursively as long as any of the units on the right hand side of Equation (15) are not SI or user-defined base units. The resulting expansion

can be simplified by combining multiplier and prefix terms to give an expression with the form given in Equation (17).

$$x_U \left[\mathbf{U} \right] = m_t \left[\frac{\mathbf{U}}{\mathbf{u}_{\mathrm{A1}}^{\mathbf{e}_{\mathrm{A1}}} \dots \mathbf{u}_{\mathrm{Zn}}^{\mathbf{e}_{\mathrm{Zn}}}} \right] x_Z \left[\mathbf{u}_{\mathrm{A1}}^{\mathbf{e}_{\mathrm{A1}}} \dots \mathbf{u}_{\mathrm{Zn}}^{\mathbf{e}_{\mathrm{Zn}}} \right]$$
(17)

 u_{II} corresponds to the units referenced by the *i*-th units definition referenced in the *I*-th definition to be expanded, and m_t is given by Equation (18).

$$m_t = m_{A1} \dots m_{Zn} p_{A1}^{e_{A1}} \dots p_{Zn}^{e_{Zn}}$$
 (18)

 m_{Ii} , p_{Ii} and e_{Ii} correspond to the values of the **multiplier**, **prefix** and **exponent** attributes on the *i*-th **<unit>** element in the *I*-th definition to be expanded.

C.3.5 Conversion between units definitions

This section presents an algorithm that specifies a possible method for converting a variable's value from one set of units to another. An example demonstrating the use of this algorithm is given in Appendix C.4.3.

If the two variable declarations that are to be mapped both reference equivalent units definitions as defined in Appendix C.2.1, then there is a one-to-one mapping between the variable's value in both components.

If the two variable declarations that are to be mapped reference different units definitions, then software may choose to calculate a conversion formula as follows. Given a variable x with units U_x , the value of which is to be passed to a variable y with units U_y , the following steps should be followed:

1. The units definitions for $\mathbf{U}_{\mathbf{x}}$ and $\mathbf{U}_{\mathbf{y}}$ are fully expanded and simplified according to the algorithm presented in Appendix C.3.4. This yields expressions for x and y in terms of x_n and y_n , the units of which are products of only SI and user-defined base units. The expression for x will be of the form given in Equation (19) if $\mathbf{U}_{\mathbf{x}}$ is a simple units definition, or of the form given in Equation (20) if $\mathbf{U}_{\mathbf{x}}$ is a complex units definition.

$$x\left[\mathbf{U}_{\mathbf{x}}\right] = m_t \left[\frac{\mathbf{U}_{\mathbf{x}}}{\mathbf{u}_{\mathbf{x}}}\right] x_n\left[\mathbf{u}_{\mathbf{x}}\right] + o_t\left[\mathbf{U}_{\mathbf{x}}\right]$$
(19)

$$x\left[\mathbf{U}_{\mathbf{x}}\right] = m_t \left[\frac{\mathbf{U}_{\mathbf{x}}}{\mathbf{u}_{\mathbf{x}}}\right] x_n\left[\mathbf{u}_{\mathbf{x}}\right]$$
(20)

In Equation (19), $\mathbf{u}_{\mathbf{x}}$ corresponds to the base units referenced in the full expansion of $\mathbf{U}_{\mathbf{x}}$, whereas in Equation (20), $\mathbf{u}_{\mathbf{x}}$ corresponds to the product of all of the base units in the full expansion raised to the appropriate exponents.

- 2. It should be considered an error if the units for $x_n(\mathbf{u}_x)$ and $y_n(\mathbf{u}_y)$ do not have equivalent dimensions as defined in Appendix C.2.2.
- 3. The expansion of x is inverted to give an expression for x_n . The inverted forms of Equation (19) and Equation (20) are given in Equation (21) and Equation (22), respectively.

$$x_{n} \left[\mathbf{u}_{\mathbf{x}} \right] = \frac{1}{m_{t}} \left[\frac{\mathbf{u}_{\mathbf{x}}}{\mathbf{U}_{\mathbf{x}}} \right] \left(x \left[\mathbf{U}_{\mathbf{x}} \right] - o_{t} \left[\mathbf{U}_{\mathbf{x}} \right] \right)$$
(21)

$$x_n \left[\mathbf{u}_{\mathbf{x}} \right] = \frac{1}{m_t} \left[\frac{\mathbf{u}_{\mathbf{x}}}{\mathbf{U}_{\mathbf{x}}} \right] x \left[\mathbf{U}_{\mathbf{x}} \right]$$
(22)

The appropriate expression for x_n can then be substituted for y_n in the expansion of y. This yields an equation for y in terms of x, which can be used to convert variable values.

C.3.6 Equation dimension checking

This section presents an algorithm that can be used to verify that an equation is consistent with respect to the dimensions of the units definitions referenced by all numbers and variables. An example that demonstrates the process of equation dimension checking for an equation defined in MathML and CellML is given in Appendix C.4.4.

This algorithm relies on the restrictions and behaviour of the different operators with respect to units defined in Appendix C.3.2 and Appendix C.3.3. Future versions of the specification may extend this algorithm to handle other operators. The steps in the algorithm are:

- 1. The equation is split into a tree of terms, in which each parent term is obtained by the application of a single operator to its children. The root of the tree is the entire equation, which is created by applying a relational operator (typically the equals operator) to its child terms. All other terms in the tree are created by applying arithmetic operators to child terms.
- 2. The units definitions for the terms at the leaves of the tree (which will be variables, numbers, or MathML constants elements) are expanded into functions of the SI and user-defined base units, using the algorithm presented in Appendix C.3.4.
- 3. Starting at the leaves of the tree, sets of child terms are recursively removed from the tree and units assigned to the parent terms. The removal of each set of terms follows the following steps:
 - (a) The child terms are compared against the restrictions described in Appendix C.3.2 for the current operator. It should be considered an error if they do not satisfy these restrictions, in which case the equation has inconsistent dimensions.
 - (b) Units are assigned to the parent term as defined in Appendix C.3.3 for the current operator.
- 4. The equation has self-consistent dimensions if no inconsistencies were found during the recursive removal of child terms during the traversal from leaves to root.

C.4 Examples

C.4.1 User-defined units and new base units

In Figure 18, the example units definitions given in <u>Section 5.3</u>¹³ are reproduced. These examples are used in the subsequent advanced examples.

C.4.2 Expansion of user-defined units

In this section, the expansion of user-defined units according to the algorithm described in Appendix C.3.4 is demonstrated for each of the units definitions given in Figure 18.

The first **<units** element in Figure 18 defines units named **pH**, and defines a **base_units** attribute with a value of "yes". This indicates that it should be treated by processing software as if it were an SI base unit, and that it cannot be expanded.

The definition of **inch** in Figure 18 is a simple units definition as it references only a single unit with an exponent of one. When the appropriate terms are substituted into Equation (??), the conversion from **metre** to **inch** is given by Equation (23). **metre** is a SI base unit, so no further expansion is necessary.

¹³http://www.cellml.org/public/specification/cellml_specification.html#sec_units_examples

```
<!-- User-defined Base Units -->
<units name="pH" base_units="yes" />
<!-- Simple Units Definitions -->
<units name="inch">
  <unit multiplier="2.54" prefix="centi" units="metre" />
</units>
<units name="fahrenheit">
  <unit multiplier="1.8" units="celsius" offset="32.0" />
</units>
<!-- Complex Units Definitions -->
<units name="celsius_per_centimetre">
  <unit units="celsius" />
  <unit prefix="centi" units="metre" exponent="-1" />
</units>
<units name="fahrenheit per inch">
  <unit units="fahrenheit" />
  <unit units="inch" exponent="-1" />
</units>
<units name="pH_per_celsius">
  <unit units="pH" />
  <unit units="celsius" exponent="-1" />
</units>
```

FIGURE 18: Some examples of the use of the **<units>** element demonstrating the definition of simple and complex units.

$$x_{new} [\text{ inch }] = \left(2.54 \ 10^{-2} \right) \left[\frac{\text{inch}}{\text{metre}} \right] x_{old} [\text{ metre }]$$

$$= 0.0254 \left[\frac{\text{inch}}{\text{metre}} \right] x_{old} [\text{ metre }]$$
(23)

The definition of **fahrenheit** is in terms of **celsius**, which is an SI derived unit. The expansion from **celsius** to **kelvin**, an SI base unit, is obtained from Section 2.1.1.5 of the SI standard, and is given in Equation (24).

$$x_{new} \left[\text{ celsius } \right] = 1.0 \left[\frac{\text{celsius}}{\text{kelvin}} \right] x_{old} \left[\text{ kelvin } \right] - 273.15 \left[\text{ celsius } \right]$$
(24)

The first step in the expansion of the **fahrenheit** definition is given in Equation (25).

$$x_f \left[\text{ fahrenheit} \right] = 1.8 \left[\frac{\text{fahrenheit}}{\text{celsius}} \right] x_c \left[\text{ celsius} \right] + 32.0 \left[\text{ fahrenheit} \right]$$
(25)

The x_c term can be replaced with the expansion of the **celsius** definition from Equation (24), as shown in Equation (26).

$$x_{f}\left[\text{ fahrenheit }\right] = 1.8 \left[\frac{\text{fahrenheit}}{\text{celsius}}\right] \left(1.0 \left[\frac{\text{celsius}}{\text{kelvin}}\right] x_{k}\left[\text{ kelvin }\right] - 273.15\left[\text{ celsius }\right]\right) + 32.0\left[\text{ fahrenheit }\right]$$
(26)

The 1.0 and 273.15 terms can be multiplied by the 1.8. The units on the resulting terms are the products of the units on the operands, as described in Appendix C.3.3, and these can be simplified according to the rules given in Appendix C.3.1. The final expansion of fahrenheit is given in Equation (27)

$$x_{f} [\text{fahrenheit}] = 1.8 \left[\frac{\text{fahrenheit}}{\text{kelvin}} \right] x_{k} [\text{kelvin}] - 491.67 [\text{fahrenheit}] + 32.0 [\text{fahrenheit}] = 1.8 \left[\frac{\text{fahrenheit}}{\text{kelvin}} \right] x_{k} [\text{kelvin}] - 459.67 [\text{fahrenheit}]$$
(27)

celsius_per_centimetre is the first of the complex units definitions given in Figure 18. The first step in the expansion of this definition is given by Equation (28), which is obtained by substituting the appropriate terms in Equation (??).

$$x_{new} \left[\text{ celsius_per_centimetre} \right] = \left(10^{-2} \right)^{-1} \left[\frac{\text{celsius_per_centimetre}}{\text{celsius metre}^{-1}} \right] x_{old} \left[\text{ celsius metre}^{-1} \right]$$
(28)

The expansion of the x_{old} term, which has units that are a product, is not obvious. This term must be expanded to continue. **metre** is an SI base unit, so need not be expanded. However, **celsius** is an SI derived unit, the expansion of which is given in Equation (24). Because this expansion is to be substituted into a complex units definition, the offset term is dropped. The next step in the expansion makes use of the modified celsius definition in Equation (29) and the identity in Equation (30).

$$v_{new} [\text{ celsius }] = 1.0 \left[\frac{\text{celsius}}{\text{kelvin}} \right] v_{old} [\text{ kelvin }]$$
(29)

$$y_{new} \left[\text{ metre}^{-1} \right] = 1.0 \left[\frac{\text{metre}^{-1}}{\text{metre}^{-1}} \right] y_{old} \left[\text{ metre}^{-1} \right]$$
(30)

The result of multiplying Equation (30) and Equation (29) is given in Equation (31).

$$v_{new} \left[\text{ celsius } \right] y_{new} \left[\text{ metre}^{-1} \right] = 1.0 \left[\frac{\text{celsius}}{\text{kelvin}} \right] v_{old} \left[\text{ kelvin } \right] 1.0 \left[\frac{\text{metre}^{-1}}{\text{metre}^{-1}} \right] y_{old} \left[\text{ metre}^{-1} \right]$$
(31)

The v_{new} and y_{new} variables can be multiplied together to produce a new unknown z_{new} which has units which are the product of the units on v_{new} and y_{new} . Similarly z_{old} is the product of v_{old} and y_{old} . The result is given in Equation (32), where the scale factors have also been multiplied.

$$z_{new} \left[\text{ celsius metre}^{-1} \right] = 1.0 \left[\frac{\text{celsius metre}^{-1}}{\text{kelvin metre}^{-1}} \right] z_{old} \left[\text{ kelvin metre}^{-1} \right]$$
(32)

 z_{new} from Equation (32) can be substituted in place of Equation (28), and the result simplified to give the complete expansion of **celsius_per_centimetre** shown in Equation (33).

$$x_{new} \left[\text{ celsius_per_centimetre } \right] = \left(10^{-2} \right)^{-1} \left[\frac{\text{celsius_per_centimetre}}{\text{celsius metre}^{-1}} \right] x_{old} \left[\text{ celsius metre}^{-1} \right]$$
$$= 100.0 \left[\frac{\text{celsius_per_centimetre}}{\text{celsius metre}^{-1}} \right] 1.0 \left[\frac{\text{celsius metre}^{-1}}{\text{kelvin metre}^{-1}} \right] z_{old} \left[\text{kelvin metre}^{-1} \right]$$
$$= 100.0 \left[\frac{\text{celsius_per_centimetre}}{\text{kelvin metre}^{-1}} \right] z_{old} \left[\text{kelvin metre}^{-1} \right]$$
(33)

The definition of **fahrenheit_per_inch** can be handled in the same way. The first step in the expansion is given by Equation (34).

$$x_{new} \left[\text{ fahrenheit_per_inch} \right] = 1.0 \left[\frac{\text{fahrenheit_per_inch}}{\text{fahrenheit inch}^{-1}} \right] x_{old} \left[\text{ fahrenheit inch}^{-1} \right]$$
(34)

The expansion of x_{old} requires the removal of the offset from the expansion of **fahrenheit** from Equation (27) and the inversion of the expansion of **inch** from Equation (23). These are given in Equation (35) and Equation (36), respectively.

$$v_{new}$$
 [fahrenheit] = 1.8 $\left[\frac{\text{fahrenheit}}{\text{kelvin}}\right] v_{old}$ [kelvin] (35)

$$y_{new}\left[\operatorname{inch}^{-1}\right] = 39.370 \left[\frac{\operatorname{inch}^{-1}}{\operatorname{metre}^{-1}}\right] y_{old}\left[\operatorname{metre}^{-1}\right]$$
(36)

Multiplying Equation (35) and Equation (36) and simplifying yields Equation (37).

$$z_{new} \left[\text{ fahrenheit inch}^{-1} \right] = 70.866 \left[\frac{\text{fahrenheit inch}^{-1}}{\text{kelvin metre}^{-1}} \right] z_{old} \left[\text{kelvin metre}^{-1} \right]$$
(37)

 z_{new} from Equation (37) can be substituted into Equation (34) in place of x_{old} and the result simplified to give the complete expansion of **fahrenheit_per_inch** in Equation (38).

$$x_{new} \left[\text{ fahrenheit_per_inch} \right] = 1.0 \left[\frac{\text{fahrenheit_per_inch}}{\text{fahrenheit inch^{-1}}} \right] x_{old} \left[\text{ fahrenheit inch^{-1}} \right]$$
$$= 1.0 \left[\frac{\text{fahrenheit_per_inch}}{\text{fahrenheit inch^{-1}}} \right] 70.866 \left[\frac{\text{fahrenheit inch^{-1}}}{\text{kelvin metre^{-1}}} \right] z_{old} \left[\text{ kelvin metre^{-1}} \right]$$
$$= 70.866 \left[\frac{\text{fahrenheit_per_inch}}{\text{kelvin metre^{-1}}} \right] z_{old} \left[\text{ kelvin metre^{-1}} \right]$$
(38)

The first step in the expansion of **pH_per_celsius** is given in Equation (39).

$$x_{new} \left[\text{ pH_per_celsius} \right] = 1.0 \left[\frac{\text{pH_per_celsius}}{\text{pH celsius}^{-1}} \right] x_{old} \left[\text{ pH celsius}^{-1} \right]$$
(39)

When user-defined base units are referenced in a simple or complex units definition, they are treated in the same way as SI base units, and not expanded. The final expansion into a combination of user-defined and SI base units is given in Equation (40).

$$x_{new} \left[\text{ pH_per_celsius} \right] = 1.0 \left[\frac{\text{pH_per_celsius}}{\text{pH kelvin}^{-1}} \right] x_{old} \left[\text{ pH kelvin}^{-1} \right]$$
(40)

C.4.3 Conversion between units definitions

In this section, the algorithm defined in Appendix C.3.5 for converting a variable's value from one set of units to another is presented with respect to a practical example. Figure 19 contains part of a CellML model definition, consisting of two components and one connection. The **legacy_imperial** component defines a variable **x** with units of **fahrenheit_per_inch**. The **modern_si** component defines a variable **y** with units of **celsius_per_centimetre**. A connection between the two components maps **x** to **y**.

```
<component name="legacy_imperial">
    <variable name="x" public_interface="out" units="fahrenheit_per_inch" />
</component>
<component name="modern_si">
    <variable name="y" public_interface="in" units="celsius_per_centimetre" />
</component>
<connection>
    <map_components component_1="legacy_imperial" component_2="modern_si" />
    <map_variables variable_1="x" variable_2="y" />
</connection>
```

FIGURE 19: In this model fragment, a connection maps a variable **x** with units of **fahrenheit_per_inch** to a variable **y** with units of **celsius_per_centimetre**.

The CellML definitions of both **fahrenheit_per_inch** and **celsius_per_centimetre** are given in Figure 18. It was shown how to obtain expressions that relate each of these units definitions to the SI base units in Appendix C.4.2. These expressions are reproduced in Equation (41) and Equation (42), respectively.

$$x_{fpi} \left[\text{ fahrenheit_per_inch} \right] = 70.866 \left[\frac{\text{fahrenheit_per_inch}}{\text{kelvin metre}^{-1}} \right] w_{kpm} \left[\text{ kelvin metre}^{-1} \right]$$
(41)

 y_{cpcm} [celsius_per_centimetre] = 100.0 $\left[\frac{\text{celsius_per_centimetre}}{\text{kelvin metre}^{-1}}\right] z_{kpm}$ [kelvin metre⁻¹] (42)

The value of x is transferred to the variable y in the mapping. Therefore an equation expressing **celsius_per_centimetre** in terms of **fahrenheit_per_inch** is needed. This can be obtained by

rearranging Equation (41) for w_{kpm} , substituting the resulting expression in place of z_{kpm} in Equation (42), and simplifying the result according to the rules defined in Appendix C.3.1. This gives the expression in Equation (43).

$$y_{cpcm} [\text{ celsius_per_centimetre }] = 100.0 \left[\frac{\text{celsius_per_centimetre}}{\text{kelvin metre}^{-1}} \right] z_{kpm} [\text{ kelvin metre}^{-1}]$$

$$= \frac{100.0 \left[\frac{\text{celsius_per_centimetre}}{\text{kelvin metre}^{-1}} \right]}{70.866 \left[\frac{\text{fahrenheit_per_inch}}{\text{kelvin metre}^{-1}} \right]} x_{fpi} [\text{ fahrenheit_per_inch }] \quad (43)$$

$$= 1.411 \left[\frac{\text{celsius_per_centimetre}}{\text{fahrenheit_per_inch}} \right] x_{fpi} [\text{ fahrenheit_per_inch }]$$

C.4.4 Equation dimension checking

In this section, the algorithm defined in Appendix C.3.6 for checking that an equation has consistent units is presented with respect to a practical example. Figure 20 contains the definition of a CellML component sodium_channel_m_gate. This component defines three sets of units (per_millisecond, millivolt, and per_millivolt), two variables (V and alpha_m) and an equation that calculates the value of alpha_m.

Equation (44) gives the equation in Figure 20, where units have been omitted. Equation (45) gives the same equation, with the units associated with each number and variable are included. The first 1.0 in the equation is included specifically for units consistency. It would be possible to associate more complex units with the 0.1 in the numerator of the equation, but this would not accurately reflect the intent of the original model authors. CellML processing software is free to find this and similar terms that do not affect the mathematics and ignore them when interpreting the equation.

$$alpha_m = 1.0 \left(\frac{0.1 \left(V + 25.0 \right)}{\exp \left(0.1 \left(V + 25.0 \right) \right) - 1.0} \right)$$
(44)

$$alpha_m [per_millisecond] = 1.0 [per_millisecond] \cdot \left(\frac{0.1 [per_millivolt] (V[millivolt] + 25.0 [millivolt])}{\exp (0.1 [per_millivolt] (V[millivolt] + 25.0 [millivolt])) - 1.0 [dimensionless]} \right)$$
(45)

The first step in the algorithm proposed in Appendix C.3.6 for verifying that a given equation has consistent dimensions is to convert the equation into a tree of equation parts. Equation (45) can be broken up into the tree shown in Figure 21.

At each branch in the tree, a single operator is applied to the child nodes, combining them into a larger parent equation part. Each equation part in the tree has units associated with it. In the case of leaf nodes, these units are obtained from the MathML equation definition. Parent nodes have units defined by the operator and the units on their child nodes, as described in Appendix C.3.3. Dimension checking begins at the leaf nodes, which are recursively removed as the units are evaluated for their parent nodes, which in turn become leaf nodes, as described in Appendix C.3.6.

In the equation tree diagram in Figure 21, the application of each operator to a set of child nodes is denoted by a number in square brackets, where the number reflects the order in which the operations are processed. These operations are discussed below.

```
<component name="sodium_channel_m_gate">
  <units name="per_millisecond">
    <unit prefix="milli" units="second" exponent="-1" />
  </units>
  <units name="millivolt">
    <unit prefix="milli" units="volt" />
  </units>
  <units name="per_millivolt">
    <unit prefix="milli" units="volt" exponent="-1" />
  </units>
  <variable name="V" units="millivolt" />
  <variable name="alpha_m" units="per_millisecond" />
  <math xmlns="http://www.w3.org/1998/Math/MathML">
    <apply><eq />
      <ci>> alpha_m </ci>
      <apply><times />
        <cn cellml:units="per_millisecond"> 1.0 </cn>
        <apply><divide />
          <apply><times />
            <cn cellml:units="per_millivolt"> 0.1 </cn>
            <apply><plus />
              <ci> V </ci>
              <cn cellml:units="millivolt"> 25.0 </cn>
            </apply>
          </apply>
          <apply><minus />
            <apply><exp />
              <apply><times />
                <cn cellml:units="per_millivolt"> 0.1 </cn>
                <apply><plus />
                  <ci> V </ci>
                  <cn cellml:units="millivolt"> 25.0 </cn>
                </apply>
              </apply>
            </apply>
            <cn cellml:units="dimensionless"> 1.0 </cn>
          </apply>
        </apply>
      </apply>
    </apply>
  </component>
```

FIGURE 20: Parts of the CellML definition of the Hodgkin Huxley squid axon model. The **sodium_channel_m_gate** component defines three sets of units, two variables **v** and **alpha_m**, and the calculation of **alpha_m**.

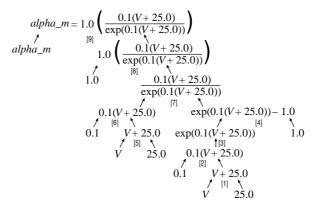


FIGURE 21: The tree form of Equation (45), in which each non-leaf node is obtained by the application of a single operator to its children. Each operator is represented by a number in square brackets. The effect of each operator is discussed in the text.

- The <plus> operator combines the variable "V" and the number "25.0" that occur in the denominator of the fraction in Equation (45). The <plus> operator requires all of its operands to be dimensionally equivalent, as described in Appendix C.2.2. The resulting equation part will have the same units as the operands. Both "V" and "25.0" have units of millivolt, and so the parent equation part "V + 25.0" also has units of millivolt.
- 2. The **<times>** operator (which is not explicitly rendered in Equation (45)) multiplies the "V + 25.0" term that is the result of the first operation by the number "0.1" which has units of **per_millivolt**. The **<times>** operator can be applied to any operands, independent of their units, and the resulting equation part has units that are the product of the units on the operands. In this case, the resultant "0.1(V + 25.0)" term has units that are the product of **millivolt** and **per_millivolt**, which simplifies to **dimensionless** (as described in Appendix C.3.1).
- 3. The **<exp>** operator is a unary arithmetic operator and its operand must have units of **dimensionless**. The result of applying the operator, in this case "exp(0.1(V + 25.0))", also has units of **dimensionless**.
- 4. The **<minus>** operator subtracts the number "1.0", which has units of **dimensionless**, from the term resulting from operation 3. The **<minus>** operator requires both its operands to have the same units and the result assumes those units.
- 5. The **<plus>** operator is applied to the variable "*V*" and the number "25.0" from the numerator of the fraction in Equation (45). Units are handled as in operation 1.
- 6. Exactly as in operation 2, where the operands are now in the numerator of the fraction in Equation (45).
- 7. The <divide> operator is applied to the results of operations 6 and 4, which both have units of dimensionless. The <divide> operator can be applied to any operands, independent of their units, and the result has the quotient of the units on the operands. In this case, the resulting fraction has units of dimensionless.
- 8. The **<times>** operator is applied to the number "1.0", which has units of **per_millisecond** and the result of operation 7, which has units of **dimensionless**. The resulting term has units of **per_millisecond**.
- 9. Finally, the **<equals>** operator is applied to the variable "*alpha_m*" and the term resulting from operation 8. The **<equals>** operator requires that its operands have dimensionally equivalent units.

D Changes

D.1 Changes between the 10 August 2001 Recommendation and the 6 November 2002 Draft

Editorial Changes

- Specification Wide¹⁴
 - The Bioengineering Research Group at the University of Auckland is now the Bioengineering Institute.
 - Several minor editorial changes have been made to all sections of the specification.
- Section 3.2.2: Definition of components¹⁵
 - Further clarified the following sentence to indicate that the name attribute need only be unique amongst all <component> elements in the current model: "Each <component> must have a name attribute, the value of which is a unique identifier for the component within the current model."
- <u>Section 3.3: Examples</u>¹⁶
 - Corrected the MathML equation in Figure 4.
- Section 3.4.6: The <map_variables> element¹⁷
 - A variable with a private_interface attribute of "in" must be mapped to a single variable owned by a component in the encapsulated set, provided the target variable has a public_interface attribute value of "out".
- Section 4.3: Examples¹⁸
 - Figure 6 has three units definitions, not two.
- Section 5.2.7: Equation dimension checking¹⁹
 - Spelling error: interoperability.
- Section 7.5.1: Implications of the **reversible** attribute²⁰
 - Added the clarifying sentence, "No assumptions must be made of the species acting in other roles."
- Section 8: Metadata Framework²¹

 $^{^{14}}http://www.cellml.org/public/specification/20021106/cellml_specification.html$

¹⁵http://www.cellml.org/public/specification/20021106/cellml_specification.html#sec_structure_component_element

¹⁶http://www.cellml.org/public/specification/20021106/cellml_specification.html#sec_structure_examples

¹⁷http://www.cellml.org/public/specification/20021106/cellml_specification.html#sec_structure_spec_rules_map_variables_element

¹⁸http://www.cellml.org/public/specification/20021106/cellml_specification.html#sec_math_examples

¹⁹http://www.cellml.org/public/specification/20021106/cellml_specification.html#sec_units_equation_dimension_checking

²⁰http://www.cellml.org/public/specification/20021106/cellml_specification.html#sec_rxn_reversible_attribute

²¹http://www.cellml.org/public/specification/20021106/cellml_specification.html#sec_metadata

- The W3C RDF Core Working Group published a new document in December of 2001 updating RDF syntax (<u>RDF/XML Syntax Specification (Revised)</u>²²). The new working draft recommends that all attributes belonging to the RDF namespace be clarified with the prefix associated with the RDF namespace (with the rdf prefix in this document). Thus, all about attributes have been given the rdf prefix.
- Corrected minor grammatical errors in Sections 8.4.1 and 8.4.2.

Changes to the Language

- Specification Wide²³
 - CellML Namespace updated to include changes. All CellML elements have been redefined under the CellML 1.1 Namespace.
- Section 1.2: Structure of the CellML Specification²⁴
 - Added Section 9 abstract.
- Section 2.2.1: Definition of a valid CellML identifier²⁵
 - Added restriction that an identifier must not begin with a digit.
- Section 2.2.2: Namespaces in CellML²⁶
 - Added XLink namespace for use with model import.
- Section 2.4.1: Valid CellML identifiers²⁷
 - Added restriction that an identifier must not begin with a digit.
- Section 3.2.1: Definition of a model²⁸
 - Changed text to correspond with new import features and recent ideas of component re-use.
 - Added <import_model> element.
- <u>Section 3.2.2</u>: Definition of components²⁹
 - Changed text to correspond with new import features and recent ideas of component re-use.
- <u>Section 3.2.3</u>: Definition of variables³⁰
 - Added description of the **units_model** attribute.

²⁸http://www.cellml.org/public/specification/20021106/cellml_specification.html#sec_structure_model_element

²²http://www.w3.org/TR/rdf-syntax-grammar/

²³http://www.cellml.org/public/specification/20021106/cellml_specification.html

²⁴http://www.cellml.org/public/specification/20021106/cellml_specification.html#sec_intro_spec_structure

²⁵http://www.cellml.org/public/specification/20021106/cellml_specification.html#sec_fundamentals_identifiers

²⁶http://www.cellml.org/public/specification/20021106/cellml_specification.html#sec_fundamentals_namespaces

²⁷http://www.cellml.org/public/specification/20021106/cellml_specification.html#sec_fundamentals_rules_identifiers

²⁹http://www.cellml.org/public/specification/20021106/cellml_specification.html#sec_structure_component_element

³⁰http://www.cellml.org/public/specification/20021106/cellml_specification.html#sec_structure_variable_element

- Section 3.2.4: Definition of connections³¹
 - Added description of the **model_1** and **model_2** attributes.
- Section 3.4.1: The **<model>** element³²
 - Added <import_model> element.
- Section 3.4.3: The **<variable>** element³³
 - Added the **units_model** attribute.
 - Expanded the allowed values of the initial_value attribute to include the value of a name attribute of a <variable> element declared in the current component.
- Section 3.4.5: The <map_components> element³⁴
 - Added the **model_1** and **model_2** attributes.
 - Expanded the proper use of the component_1 and component_2 attributes to include the model_1 and model_2 attributes.
- Section 5.2.2: User defined units³⁵
 - Added the **units_model** attribute.
- Section 5.4.2: The **<unit>** element³⁶
 - Added the **units_model** attribute.
- Section 9: Importing Models³⁷
 - Newly added to specify the import feature.
- Appendix A.6: The CellML DTD³⁸
 - Incorporates the changes listed above.
 - Made the relationship attribute on the <relationship_ref> element optional because the relationship attribute can be placed under a user-defined namespace and still be valid CellML.

D.2 Changes between 18 May 2001 Final Draft and the 10 August 2001 Recommendation

The full list of changes made between the 18 May 2001 Final Draft and the 10 August 2001 Recommendation of the CellML 1.0 specification can be found at Appendix D of the 10 August 2001 Recommendation³⁹.

³⁴http://www.cellml.org/public/specification/20021106/cellml_specification.html#sec_structure_spec_rules_map_components_element

³¹http://www.cellml.org/public/specification/20021106/cellml_specification.html#sec_structure_connection_element

³²http://www.cellml.org/public/specification/20021106/cellml_specification.html#sec_structure_spec_rules_model_element

 $^{^{33}} http://www.cellml.org/public/specification/20021106/cellml_specification.html \\ \texttt{\#sec_structure_spec_rules_variable_element}$

³⁵http://www.cellml.org/public/specification/20021106/cellml_specification.html#sec_units_user_defined_units

³⁶http://www.cellml.org/public/specification/20021106/cellml_specification.html#sec_units_spec_rules_unit_element

³⁷http://www.cellml.org/public/specification/20021106/cellml_specification.html#sec_import_model

³⁸http://www.cellml.org/public/specification/20021106/cellml_specification.html#sec_cellml_1_1_dtd

³⁹http://www.cellml.org/public/specification/20010810/cellml_specification.html#changes

D.3 Changes between 2 March 2001 Draft and the 18 May 2001 Final Draft

The complete list of changes made between the 2 March 2001 Draft and the 18 May 2001 Final Draft of the CellML 1.0 specification can be found at Appendix D of the 18 May 2001 Final Draft⁴⁰.

E-mail questions, criticism, submissions or info to info@cellml.org Input document last modifi ed : Thu Oct 30 16:04:30 NZDT 2003

⁴⁰http://www.cellml.org/public/specification/20010518/cellml_specification.html#sec_changes